### **Accepted Manuscript**

On the cohesion of fluids and their adhesion to solids: Young's equation at the atomic scale

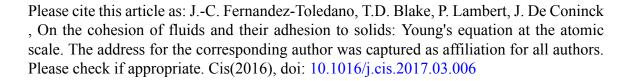
J.-C. Fernandez-Toledano, T.D. Blake, P. Lambert, J. De Coninck

PII: S0001-8686(16)30324-4

DOI: doi: 10.1016/j.cis.2017.03.006

Reference: CIS 1731

To appear in: Advances in Colloid and Interface Science



This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



## **ACCEPTED MANUSCRIPT**

# On the cohesion of fluids and their adhesion to solids: Young's equation at the atomic scale

J-C. Fernandez-Toledano<sup>a1</sup>, T. D. Blake<sup>a</sup>, P. Lambert<sup>b</sup>, and J. De Coninck<sup>a</sup> *Laboratory of Surface and Interfacial Physics (LPSI), University of Mons, 7000 Mons, Belgium* 

#### **Abstract**

Using large-scale molecular dynamics simulations, we model a 9.2 nm liquid bridge between two solid plates having a regular hexagonal lattice and analyse the forces acting at the various interfaces for a range of liquid-solid interactions. Our objective is to study the mechanical equilibrium of the system, especially that at the three-phase contact line. We confirm previous MD studies that have shown that the internal pressure inside the liquid is given precisely by the Laplace contribution and that the solid exerts a global force at the contact line in agreement with Young's equation, validating it down to the nanometre scale, which we quantify. In addition, we confirm that the force exerted by the liquid on the solid has the expected *normal* component equal to  $\gamma_{lv} \sin \theta^0$ , where  $\gamma_{lv}$  is the surface tension of the liquid and  $\theta^0$  is the equilibrium contact angle measured on the scale of the meniscus. Recent thermodynamic arguments predict that the *tangential* force exerted by the liquid on the solid should be equal to the work of adhesion expressed as  $Wa^0 = \gamma_{lv} (1 + \cos \theta^0)$ . However, we find that this is true only when any layering of the liquid molecules close to liquid-solid interface is negligible. The force significantly exceeds this value when strong layering is present.

Keywords: Wetting, adhesion, three-phase contact zone, liquid-solid interface, molecular-dynamics

#### **Contents**

- 1. Introduction
- 2. Simulations
- 3. Forces on the liquid
- 4. Forces on the solid
- 5. Conclusions

Acknowledgements

References

Corresponding author

\_

<sup>&</sup>lt;sup>b</sup> Université libre de Bruxelles - BEAMS CP165/56 - Av. F.D. Roosevelt 50 - B1050 Bruxelles

### Download English Version:

## https://daneshyari.com/en/article/4981439

Download Persian Version:

https://daneshyari.com/article/4981439

<u>Daneshyari.com</u>